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The report describes progress on diffusion studies in Mercury Cadmium Telluride and on growth studies in Mercury Cadmium Telluride. The former emphasizes self-diffusion (isoconcentration or tracer diffusion) measurements, interdiffusion measurements, and the analysis of the relationship between the self-diffusion coefficients and the interdiffusion coefficients for pseudo-binary systems. The growth studies concern the characterization of isothermal vapor phase epitaxial MCT layers (ISOVPE) using defect etching and Rutherford backscattering methods (RBS).

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"Diffusion and Defect Characterization Studies of Mercury Cadmium Telluride"

Principal Investigator: D. A. Stevenson

Department of Materials Science and Engineering
Stanford University
Stanford, CA 94305

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I. Progress During the Report Period

During the last six month period, progress has continued in two major areas of this program: diffusion studies in Mercury Cadmium Telluride (MCT); and growth studies in MCT. The diffusion studies in the present report period concern the self-diffusion (isoconcentration or tracer diffusion) measurements, interdiffusion measurements, and the analysis of the relationship between the self-diffusion coefficients and the interdiffusion coefficients for pseudo-binary systems. The growth studies concern the characterization of isothermal vapor phase epitaxial MCT layers (ISOVPE) using defect etching and Rutherford backscattering methods (RBS). Two papers have been submitted for publication, both concerning interdiffusion in MCT. A description of our activity in the last report period is given below.

A. Diffusion Studies

Progress has continued on the measurement of component tracer diffusion coefficients in MCT, further analysis of the interdiffusion behavior in MCT, and on the development of fundamental equations relating self-diffusion coefficients to the interdiffusion coefficients in pseudo-binary systems. Component tracer diffusion measurements have been completed and we are presently developing defect models based on available defect concentration information and an analysis of the correlation factor in pseudo-binary systems. Basic governing equations have been derived from theory to calculate interdiffusion coefficients from the component self-diffusion coefficients in the MCT pseudo-binary system. These relationships explain the observed behavior that $D((X=0.2)=D_{Cd}^{*}(X=0.2)$, where D_{Cd}^{*} is the slower self-diffusion coefficient of the two metal species. (X is the CdTe mole fraction in MCT.) The theory for the pseudo-binary system is based on fundamental constraints for a pseudo-binary system, namely, the Gibbs-Duhem equation for a ternary system, and additional constraints: (1) when the major diffusing species are charged, the electroneutrality condition is operative; and (2)

local defect equilibrium for the the intrinsic case. The resulting mathmatical expression is fairly complex, but it can be simplified into one of two limiting cases, depending on the relative dffusivity of metal to non-metal. This theory is not only valid for MCT systems, but for any pseudo-binary system.

B. Growth Studies

In the present program, we have studied a number of epitaxial growth methods, with particular emphasis on the ISOVPE method. We have developed a growth model for this method that is consistent with information in the literature on the thermodynamics and kinetics for the growth systmem. We have also refined many aspects of the method, particularly, the control of the surface composition (X value). The growth method is attractive for its simplicity, ease of scaleup and the exceptional surface quality of the layers. In addition, good devices have been made from this material. We are presently analyzing the inherent purity and perfection of the material using a number of charaterization methods. In our current work, we are using defect etching to determine the profile of the dislocation density from the growth interface to the layer surface and we are using RBS channelling methods to determine the perfection of the material.

We are presently evaluating ISOVPE MCT layers grown on (111)A and (111)B faces of $Cd_{1-Y}Zn_YTe$ substrates at various growth times. The relation between the dislocation density, the width of high dislocation density region, and the growth times were established by angle lapping and etching using a Polisar etch. The highest dislocation densities were at the interface of VPE layer and CdZnTe substrate with values between 10^7 and $5x10^5$. As the growth time is increased, the dislocation density and the width of high dislocation density region decreases. Dislocation densities of 10^4 were measured at the surface for as-grown layers and this is comparable to the best quality LPE layers. The quality of the layers was also evaluated using RBS techniques and this confirmed that our ISOVPE layers were comparable to the best quality LPE layers, at least in accord with these criteria.

II. Planned Activity for the Coming Period

The work planned for the future emphasizes the following topics: continuation of the analysis of the diffusion studies, with emphasis on the relationship between the different diffusion coefficients; a study of the diffusion of mercury in $Hg_{1-x}Zn_xTe$; continuation of defect studies in MCT using etching and RBS methods; electrical characterization of MCT by Van der Pauw measurements; and the preparation of graded junctions by increasing the Cd concentration on VPE grown surfaces.

III. There were no changes in the key personnel in the report period.

IV. During the report period, M. F. S. Tang and D. A. Stevenson presented a paper October 8, 1986 at The 1986 U. S. Workshop on the Physics and Chemistry of Mercury Cadmium Telluride at Dallas, Texas, and submitted two papers for publication. J. G. Fleming and D. A. Stevenson submitted two papers for publication.